Machine Learning-Enhanced Strategic Synthesis Planning

We are looking for highly motivated PhD students/PostDocs for projects at the intersection between advanced machine learning and chemistry. We will have **one fully-funded industrial position** in **summer 2023** (the earliest starting date is August 2023). Join our vibrant and dynamic team to build the synthesis planning models of the future!

Project background

Over the last hundred years, not much has changed how organic chemistry is conducted. In most laboratories, the current state is still trial-and-error experiments guided by human expertise acquired over decades. What if, given all the knowledge collected and expertise gained, we could develop machine learning-based assistants to accelerate the discovery of novel molecules and design sustainable routes incorporating green chemistry principles?

Although we currently observe a rise in machine learning approaches for chemical synthesis, they only scratch the surface of what is feasible. We want to foster close collaborations with synthetic chemists, develop approaches that can be tested experimentally, and facilitate the adoption of machine learning techniques in their daily workflows.

This project aims to develop machine learning (ML) approaches for strategic multi-step synthesis planning in chemistry. The team will create standardized synthesis datasets, develop ML models to capture synthesis strategies, and suggest benchmarks for evaluating synthesis planning tools. The ultimate goal is to advance ML for synthesis planning, provide chemists with new ideas, and accelerate the synthesis of novel, sustainable chemicals.

Your profile

- A Master degree or a four or five-year Bachelor degree in Chemistry, Chemical Engineering, Computer Science or related fields for the PhD position / a PhD in a related field for the PostDoc position

- Motivation for working on challenging projects, passion for scientific research, and thrive for excellence
- Strong teamwork and communication skills
- Growth mindset and inclusive team culture
- English proficiency
- Programming and machine learning experience (e.g. in Python)

Application and Selection Process

1. Send a CV and summary (1-2 pages) of previously done research projects to **philippe.schwaller@epfl.ch** with the subject "PhD/Postdoc in Machine Learning-Enhanced Strategic Synthesis Planning".
2. Selected candidates will be invited first to a non-technical discussion, and then in a second round to a technical interview (including a 25 minutes presentation). The top candidates will meet with the group.
3. PhD positions require acceptance to the doctoral program of Chemistry and Chemical Engineering. Becoming a PhD student at EPFL thus consists of applying at: https://www.epfl.ch/education/phd/edch-chemistry-and-chemical-engineering/edch-how-to-apply/. This page also contains additional administrative information on PhD positions at EPFL.

We look forward to receiving your application before **May 5, 2023**.

Doing a PhD at EPFL

The École Polytechnique Fédérale de Lausanne (EPFL) is a world-leading university and provides an internationally recognised, collaborative and well-funded environment. QS World University Rankings, for instance, rank EPFL in the top-10 worldwide in Chemistry and Computer Science and Information Systems. With the AI4Science initiative, EPFL has a platform to promote interdisciplinary research in artificial intelligence and machine learning and connect researchers from various fields.

EPFL is located in Lausanne, in the French speaking part of Switzerland (by train ~40 min to Geneva, ~2 hours to Zurich). Switzerland is a beautiful and safe country with great work-life balance and life satisfaction. Mountains and great outdoor activities (e.g. hiking, biking, sailing, and skiing) are never too far away.

The PhD student will be employed externally by the industrial partner in Basel to work on an existing high-throughput experimentation platform, but spend a non-negligible amount of his PhD at EPFL and benefit from the interactions with the LIAC team.

There is an excellent blog post by Mathias Payer on doing a PhD at EPFL in Computer Science. Compared to the Computer Science doctoral school with 30 required ECTS course credits, the Chemistry and Chemical Engineering one only requires 12 ECTS. The courses can be taken in chemistry or machine learning depending on your interests. Summer schools and conferences are another way to obtain ECTS credits.

For more information, check out the comprehensive "Best practices guide for doctoral studies at EPFL".

All in all, PhD is a unique opportunity to dive into a specific topic, learn new skills and grow to become an expert in the field.

Equality and Diversity

At EPFL, people from a wide range of cultural and academic backgrounds work and study together. Diversity is a strength. It requires an environment of mutual respect to allow the members of the EPFL community, individually and collectively, to achieve exceptional results.

We will encourage diversity and foster a culture of inclusion where everyone feels welcome. We will not tolerate any discrimination on grounds such as gender, sexual orientation, disability, the colour of skin, social origin, and religious affiliation.

Contact

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